

4-Aminobutanoic acid
56-12-2 | DTXSID6035106

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 266 °C

Global applicability domain: Inside

Local applicability domain index: 7.40e-01

Confidence level: 4.57e-01

Nearest Neighbors from the Training Set

Image not found

beta-Aminobutyric acid

Measured: 193

Predicted: 250

Image not found

Alanine, 2-methyl-

Measured: 335

Predicted: 307